On gauge transformations of Bäcklund type and higher order nonlinear Schrödinger equations

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Abstract

We introduce a new, more general type of nonlinear gauge transformation in nonrelativistic quantum mechanics that involves derivatives of the wave function and belongs to the class of Bäcklund transformations. These transformations satisfy certain reasonable, previously proposed requirements for gauge transformations. Their application to the Schrödinger equation results in higher order partial differential equations. As an example, we derive a general family of 6th-order nonlinear

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Schrödinger equations, closed under our nonlinear gauge group. We also introduce a new gauge invariant current $\sigma = \rho \nabla \triangle \ln \rho$, where $\rho = \bar{\psi}\psi$. We derive gauge invariant quantities, and characterize the subclass of the 6th-order equations that is gauge equivalent to the free Schrödinger equation. We relate our development to nonlinear equations studied by Doebner and Goldin, and by Puszkarz.

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1 Introduction

The notion of nonlinear gauge transformation, introduced in quantum mechanics by Doebner and Goldin, extends the usual group of unitary gauge transformations.[1−3] The resulting nonlinear transformations act on a parameterized family of nonlinear Schrödinger equations (NLSEs) that includes the linear Schrödinger equation as a special case. They are called gauge transformations because they leave invariant the outcomes of all physical measurements. In this paper we extend the notion of gauge transformation further to include transformations that depend explicitly on derivatives of the wave function. The result is a group of transformations of Bäcklund type.[4]

As described in earlier work,[3] a (nonlinear) gauge transformation is implemented by a transformation $\psi' = \mathcal{N}[\psi]$, assumed to satisfy the following conditions:

- 1. The *principle of gauge-independence of positional measurements:* Invariance is required of all quantities describing outcomes of positional measurements, including *sequences* of measurements performed successively at different times. In particular, $\rho(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2$ should be invariant under $\mathcal{N}$ for the single-particle wave function ψ.

- 2. *Strict locality:* If ψ is a single-particle function, the value of ψ' at $(\mathbf{x}, t)$ is assumed to depend only on the value of $\mathbf{x}$, the value of t, and the value of ψ at $(\mathbf{x}, t)$.

- 3. A *separation condition:* If $\psi^{(N)}$ is a wave function describing a set of N noninteracting particles (i.e., a product state), then $\psi^{(N)'}$ is well defined as the product of gauge transformed single particle wave functions. This condition ensures that gauge transformations extend to the whole N-particle hierarchy of wave functions in a way that subsystems that are uncorrelated remain so in the gauge-transformed theory.

Here we modify the condition of strict locality, allowing $\psi'(\mathbf{x}, t)$ to depend not only on the values of $\psi(\mathbf{x}, t)$, $\mathbf{x}$, and t, but also on finitely many spatial derivatives of ψ evaluated at $(\mathbf{x}, t)$. Thus our transformations are local, in that $\psi'(\mathbf{x}, t)$ does not depend on space-time points any distance from $(\mathbf{x}, t)$, but they are no longer "strictly" local, since derivative terms are allowed. We shall call this property *weak locality*. One motivation for introducing this generalization is to explore the relation between the resulting nonlinear gauge generalization of the Schrödinger equation and the equations proposed by Puszkarz.[5]

The condition that our set of transformations forms a group (i.e., that it is closed under composition and includes all inverse transformations) while the number of derivatives of ψ remains bounded, imposes an additional restriction. This *group property* is automatically satisfied in the strictly local theory, but here it requires explicit discussion. Thus, we shall add it to the conditions already mentioned. We then call the transformations that obey the following four conditions *weakly local gauge transformations*: 1. the principle of gauge-independence of positional measurements; $2'$. weak locality; 3. the separation condition; and 4. the group property.

In Sec. 2 of this paper, we first consider a general class of nonlinear, single particle Schrödinger equations that are equivalent to the free Schrödinger equation under the assumption that condition 1 is satisfied. Using the other three conditions, we obtain a particularly simple form for weakly local gauge transformations. Following the method of "gauge generalization,"[3] we then derive a general family of 6th-order nonlinear Schrödinger equations, closed under our nonlinear gauge group, which are not all equivalent to the free 2nd-order Schrödinger equation. In Sec. 3 we construct a complete set of gauge invariant quantities. As particular cases, we use these to characterize the subclass of the 6th-order equations that are gauge equivalent to the Schrödinger equation, and those equivalent to the wider class of nonlinear equations studied by Doebner and Goldin. We further relate our development to the nonlinear equations proposed by Puszkarz based on additional quantum currents that involve higher derivatives of ψ.

2 Gauge Transformations and NLSEs

Consider the transformation

$$\psi'(\mathbf{x},t) \;=\; e^{i\varphi}\psi(\mathbf{x},t), \tag{2.1}$$

where φ is a real-valued functional that depends on $\psi, \mathbf{x}$, and t. By this we mean that φ can depend explicitly on ψ, $\bar{\psi}$, derivatives of ψ and $\bar{\psi}$ of arbitrary order, integrals or integral transforms of ψ and $\bar{\psi}$, etc., as well as directly on $\mathbf{x}$ and t. Eq. (2.1) preserves the probability density $\rho(\mathbf{x},t) = \bar{\psi}(\mathbf{x},t)\psi(\mathbf{x},t)$, as required by the first condition in Sec. 1, but if nonlocal it does not generally respect sequences of positional measurements. The following then describes the general class of NLSEs that are equivalent via (2.1) to the free Schrödinger equation: if ψ' satisfies

$$i\frac{\partial\psi'}{\partial t} + \frac{\hbar}{2m}\triangle\psi' \;=\; i\frac{\partial\psi'}{\partial t} - \nu_1'\triangle\psi' = 0, \tag{2.2}$$

then ψ satisfies the NLSE

$$i\frac{\partial\psi}{\partial t} - \nu_1'\triangle\psi + iI[\psi,\mathbf{x},t]\psi + R[\psi,\mathbf{x},t]\psi = 0, \tag{2.3}$$

where

$$R[\psi,\mathbf{x},t] \;=\; \frac{\partial\varphi}{\partial t} - 2\nu_1'(\frac{\nabla\varphi\cdot\hat{\mathbf{j}}}{\rho} + \frac{1}{2}(\nabla\varphi)^2) \tag{2.4}$$

and

$$I[\psi,\mathbf{x},t] \;=\; \nu_1'(\triangle\varphi + \frac{\nabla\varphi\cdot\nabla\rho}{\rho}) \;=\; \nu_1'[\frac{1}{\rho}(\nabla\cdot(\rho\nabla\varphi)], \tag{2.5}$$

with

$$\hat{\mathbf{j}} = \frac{m}{\hbar}\mathbf{j} = \frac{1}{2i}[\bar{\psi}\nabla\psi - (\nabla\bar{\psi})\psi]. \tag{2.6}$$

The verification is by direct substitution of (2.1) into (2.2).

As was shown by Doebner and Goldin[1], a general form for strictly local gauge transformations (that satisfy all the initial requirements discussed in Sec. 1) corresponds to the choice

$$\varphi = \frac{1}{2}\gamma(t)\ln\rho + [\Lambda(t) - 1]S + \theta(\mathbf{x}, t), \quad \Lambda \neq 0, \tag{2.7}$$

where $\psi = \sqrt{\rho}\, e^{iS}$. For simplicity, we consider $\theta(\mathbf{x}, t) \equiv 0$. The family of NLSEs with arbitrary coefficients that directly generalizes (2.3) and is invariant (as a family) under gauge transformations (2.1) with φ as in (2.7), then has the form[1]

$$i\frac{\partial\psi}{\partial t} = \{i\sum_{j=1}^{2}\nu_j(t)R_j + \sum_{j=1}^{5}\mu_j(t)R_j\}\psi, \tag{2.8}$$

where

$$R_1 = \frac{\nabla\cdot\hat{\mathbf{j}}}{\rho}, \quad R_2 = \frac{\triangle\rho}{\rho}, \quad R_3 = \frac{\hat{\mathbf{j}}^2}{\rho^2}, \quad R_4 = \frac{\hat{\mathbf{j}}\cdot\nabla\rho}{\rho^2}, \quad R_5 = \frac{(\nabla\rho)^2}{\rho^2}. \tag{2.9}$$

In obtaining (2.8), one uses the identity $\triangle\psi/\psi = iR_1 + \frac{1}{2}R_2 - R_3 - \frac{1}{4}R_5$. Invariance of the family (2.8) under (2.1) and (2.7) means that if ψ satisfies an equation in this family with coefficients ν_j and μ_j, then ψ' satisfies another equation in the family with coefficients ν'_j and μ'_j; thus our choice of the primed coefficient ν'_1 in writing Eq. (2.2).

Now the class of nonlinear gauge transformations in quantum mechanics can be essentially extended if we replace strict locality by weak locality, thus allowing the gauge functional φ to depend on derivatives of ψ. Under this assumption the gauge transformation is no longer simply a point transformation; it is a *Bäcklund transformation.*[4] Here we consider gauge transformations of Bäcklund type that form a group, satisfying the physically motivated requirements discussed in Sec. 1, with strict locality replaced by weak locality.

We observe that if φ is permitted to depend on derivatives of S as well as derivatives of ρ, then the set of gauge transformations in general does not respect the group property. However, if the derivatives of S are excluded from φ, then the transformations do respect this property. One way to see this is to write nonlinear gauge transformations as they act on logarithmic coordinates T and S, with $\ln\psi = T + iS$ (so that $T = \frac{1}{2}\ln\rho$), omitting for simplicity the explicit $\mathbf{x}$ and t dependence:

$$\begin{pmatrix} S' \\ T' \end{pmatrix} = \begin{pmatrix} L & G \\ 0 & 1 \end{pmatrix} \begin{pmatrix} S \\ T \end{pmatrix}, \tag{2.10}$$

where L is a linear or nonlinear functional of S and its derivatives, and G is a linear or nonlinear functional of T and its derivatives. In the strictly local case, we have $L[S] = \Lambda S$ and $F[T] = \gamma T$. If we perform two transformations (2.10) successively, $T'' = T' = T$ and $S'' = L_2[L_1[S] + G_1[T]] + G_2[T]$. Then derivatives present in the form of G never act successively, so that their order does not increase; but derivatives in the form of L do act successively. Thus the group property, with the condition that the number of derivatives of ψ remains bounded, rules out derivative terms in L—but not in G.

Now a simple gauge transformation that is no longer strictly local, but satisfies the four requirements discussed in Sec. 1, has the form (2.1) with

$$\varphi = \frac{1}{2}\gamma\ln\rho + (\Lambda - 1)S + \eta\triangle\ln\rho = \frac{1}{2}\gamma\ln\rho + (\Lambda - 1)S + \eta(R_2 - R_5), \tag{2.11}$$

where η is a real parameter that, like γ and Λ, can in principle depend on t. This corresponds to the choice $G[T] = \gamma T + \eta\triangle T$ in (2.10). Thus we have a group of nonlinear gauge transformations modeled on three (in general time-dependent) parameters, obeying the group law

$$\mathcal{N}_{(\gamma_2,\Lambda_2,\eta_2)} \circ \mathcal{N}_{(\gamma_1,\Lambda_1,\eta_1)} = \mathcal{N}_{(\gamma_2+\Lambda_2\gamma_1,\Lambda_2\Lambda_1,\eta_2+\Lambda_2\eta_1)}. \tag{2.12}$$

But we note further that $G[T]$ need not be linear in T. Indeed, while the linear term $\triangle\ln\rho = R_2 - R_5$ satisfies the separation condition, its nonlinear parts R_2 and R_5 do so separately! Considering a two-particle product wave function $\psi^{(2)}(\mathbf{x_1},\ \mathbf{x_2},\ t) = \psi_1(\mathbf{x_1}, t)\psi_2(\mathbf{x_2}, t)$, and defining $\rho^{(2)} = \overline{\psi^{(2)}}\psi^{(2)}$, $\rho_1 = \bar{\psi}_1\psi_1$, and $\rho_2 = \bar{\psi}_2\psi_2$, we have

$$R_2^{(2)}[\psi^{(2)}] = \frac{\triangle^{(2)}\rho^{(2)}}{\rho^{(2)}} = \frac{\triangle^{(2)}(\rho_1\rho_2)}{\rho_1\rho_2} = \frac{\triangle_1\rho_1}{\rho_1}\frac{\triangle_2\rho_2}{\rho_2} = R_2[\psi_1]R_2[\psi_2],$$

where $\triangle^{(2)} = \triangle_1 + \triangle_2$. Similarly for R_5:

$$R_5^{(2)}[\psi^{(2)}] = \frac{[\nabla^{(2)}\rho^{(2)}]^2}{\left(\rho^{(2)}\right)^2} = \frac{[(\nabla_1, \nabla_2)\rho_1\rho_2]^2}{(\rho_1\rho_2)^2} = R_5[\psi_1]R_5[\psi_2].$$

Thus a further generalization of (2.11) that gives weakly local nonlinear gauge transformations is to allow the derivative terms to enter with different coefficients:

$$\varphi = \frac{1}{2}\gamma \ln \rho + (\Lambda - 1)S + \eta_1 R_2 + \eta_2 R_5. \tag{2.13}$$

Let us next write the gauge generalized family of NLSEs derived from (2.11). Beginning with the standard, free Schrödinger equation in the form

$$i\frac{\partial \psi'}{\partial t} = -\frac{\hbar}{2m}[iR_1' + (\frac{1}{2}R_2' - R_3' - \frac{1}{4}R_5')]\psi', \tag{2.14}$$

where R_j' means $R_j[\psi']$, we transform by (2.1) with φ as in (2.11), and from (2.3)-(2.5) we find the form of the resulting NLSEs for ψ. We generalize, following Ref. 3, by allowing arbitrary coefficients for the nonlinear functionals, maintaining the invariance of the family of NLSEs under the nonlinear gauge group. In this fashion, we obtain the following equations:

$$i\frac{\partial \psi}{\partial t} = \{i\sum_{j=1,2,6} \nu_j R_j + \sum_{j=1}^{12} \mu_j R_j\}\psi = \{i\hat{I} + \hat{R}\}\psi, \tag{2.15}$$

where $R_1, ..., R_5$ are as in (2.9), and where the new functionals $R_6, ..., R_{12}$ are given by:

$$R_6 = \frac{\nabla \cdot \sigma}{\rho}, \qquad R_7 = \frac{\hat{\mathbf{j}} \cdot \sigma}{\rho^2}, \qquad R_8 = \frac{\sigma \cdot \nabla\rho}{\rho^2}, \tag{2.16}$$

$$R_9 = \frac{\sigma^2}{\rho^2}, \quad R_{10} = \triangle R_1, \quad R_{11} = \triangle R_2, \quad R_{12} = \triangle R_6,$$

with

$$\sigma = \rho\nabla\triangle \ln \rho = \rho\nabla(R_2 - R_5). \tag{2.17}$$

Note that the functionals $R_6, ..., R_{11}$ involve no higher than fourth derivatives of ψ, but the presence of the term R_{12} in (2.15) makes it in general of 6th order. If we use (2.13) in place of (2.11), we shall need separately the new currents $\rho\nabla R_2$ and $\rho\nabla R_5$. These give rise to additional nonlinear functionals in ψ.

Equation (2.15) still conserves the quantum probability $\bar{\psi}\psi$ It gives rise to the gauge invariant current

$$\mathbf{J}^{gi} = -2(\nu_1 \hat{\mathbf{j}} + \nu_2 \nabla\rho + \nu_6 \sigma) \tag{2.18}$$

that enters the continuity equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}^{gi} = 2\hat{I}\rho. \tag{2.19}$$

3 Gauge transformations and invariants for the family of 6th-order NLSEs

Under the gauge transformations (2.1), with φ given by (2.11) the coefficients ν_j, μ_j of (2.15) transform as follows:

$$\nu_1' = \frac{\nu_1}{\Lambda}, \qquad \nu_2' = \nu_2 - \frac{1}{2}\gamma\frac{\nu_1}{\Lambda}, \qquad \nu_6' = \nu_6 - \frac{\eta}{\nu_1 \Lambda} \qquad (\Lambda = \lambda + 1); \tag{3.1}$$

$$\mu_1' = \mu_1 - \frac{\gamma\nu_1}{\Lambda}, \qquad \mu_2' = \Lambda\mu_2 - \frac{1}{2}\gamma\mu_1 + \frac{\gamma^2}{2\Lambda}\nu_1 - \gamma\nu_2, \qquad \mu_3' = \frac{\mu_3}{\Lambda} \tag{3.2}$$

$$\mu_4' = \mu_4 - \frac{\gamma\mu_3}{\Lambda}, \qquad \mu_5' = \Lambda\mu_5 - \frac{1}{2}\gamma\mu_4 + \frac{\gamma^2}{4\Lambda}\mu_3,$$

$$\mu_6' = \Lambda\mu_6 - \gamma\nu_6 - \eta\mu_1 + \frac{\eta\gamma}{\Lambda}\nu_1, \qquad \mu_7' = \mu_7 - \frac{2\eta\mu_3}{\Lambda}$$

$$\mu_8' = \Lambda\mu_8 - \eta\mu_4 - \frac{1}{2}\gamma\mu_7 + \frac{\gamma\eta\mu_3}{\Lambda}, \qquad \mu_9' = \Lambda\mu_9 - \eta\mu_7 + \frac{\eta^2\mu_3}{\Lambda}, \qquad \mu_{10}' = \mu_{10} - \frac{2\eta\nu_1}{\Lambda},$$

$$\mu_{11}' = \Lambda\mu_{11} - 2\eta\nu_2 - \frac{1}{2}\gamma\mu_{10} + \frac{\gamma\eta\nu_1}{\Lambda}, \qquad \mu_{12}' = \Lambda\mu_{12} - 2\eta\nu_6 - \eta\mu_{10} + \frac{2\eta^2\nu_1}{\Lambda}.$$

Note that as expected, η does not enter the transformation laws for ν_1, ν_2, or $\mu_1, ..., \mu_5$, which are the same as in Refs. 1-3. Note also that if we begin with $\mu_{12} = 0$, then $\eta \neq 0$ leads to $\mu'_{12} \neq 0$; thus we cannot have an invariant family of 4th-order partial differential equations for these transformations.

We now write functionally independent gauge invariants τ_j $(j = 1, 2, ..., 12)$ as follows:

$$\tau_1 = \nu_2 - \frac{\mu_1}{2}, \;\; \tau_2 = \nu_1\mu_2 - \mu_1\nu_2, \;\; \tau_3 = \frac{\mu_3}{\nu_1}, \;\; \tau_4 = \mu_4 - \mu_1\frac{\mu_3}{\nu_1}, \;\; \hat{\tau}_5 = \mu_5\mu_3 - (1/4)\mu_4^2, \tag{3.3}$$

$$\tau_6 = \mu_6\nu_1 - \mu_1\nu_6, \qquad \tau_7 = \mu_7 - 2\nu_6\frac{\mu_3}{\nu_1}, \qquad \tau_8 = \mu_8\nu_1 - \mu_4\nu_6 + \mu_6\mu_3 - (1/2)\mu_7\mu_1,$$

$$\tau_9 = \mu_9\mu_3 - (1/4)\mu_7^2, \;\; \tau_{10} = \mu_{10} - 2\nu_6, \;\; \tau_{11} = \mu_{11}\nu_1 - \mu_{10}\nu_2, \;\; \tau_{12} = \mu_{12}\nu_1 - \nu_6^2 - (1/4)\mu_{10}^2.$$

In this list of gauge invariants, we have included a new quantity $\hat{\tau}_5$ instead of the original $\tau_5 = \nu_1\mu_5 - \nu_2\mu_4 + \nu_2^2(\mu_3/\nu_1)$ that was used in Refs. 1-3, since the expression for $\hat{\tau}_5$ is simpler. The relation between these two gauge invariants is, of course, wholly gauge invariant: $\hat{\tau}_5 = \tau_3\tau_5 + \tau_1\tau_3(\tau_4 - \tau_1\tau_3) - (1/4)\tau_4^2 = \tau_3\tau_5 - (\tau_1\tau_3 - \frac{1}{2}\tau_4)^2$.

It should be noted that (2.15) is invariant under Galilean transformations

$$\tilde{\mathbf{x}} = \mathbf{x} - \mathbf{v}t, \;\; \tilde{t} = t, \;\; \tilde{\psi}(\tilde{\mathbf{x}}, \tilde{t}) \; = \; \psi(\mathbf{x}, t)\, e^{\frac{i}{2\nu_1}(\mathbf{x}\cdot\mathbf{v} + \frac{1}{2}v^2 t)} \tag{3.4}$$

when

$$\frac{\mu_3}{\nu_1} = -1, \;\; \mu_1 + \mu_4 = 0, \;\; \mu_7 + \mu_{10} = 0, \tag{3.5}$$

and consequently, the gauge invariants τ_1,... τ_{12} must satisfy the conditions

$$\tau_3 = -1, \quad \tau_4 = 0, \quad \tau_7 + \tau_{10} = 0. \tag{3.6}$$

Under time reversal, all the coefficients ν_j, μ_j change sign. Thus time reversal invariance requires

$$\tau_1 = 0, \quad \tau_4 = 0, \quad \tau_7 = 0, \quad \tau_{10} = 0. \tag{3.7}$$

In particular, when (2.15) is the Schrödinger equation, we have

$$\nu_1 = -\frac{\hbar}{2m}, \quad \mu_2 = -\frac{\hbar}{4m}, \quad \mu_3 = \frac{\hbar}{2m}, \quad \mu_5 = \frac{\hbar}{8m}, \tag{3.8}$$

and all other coefficients are zero. Eqs. (3.7) then give

$$\tau_2 = \frac{\hbar^2}{8m^2}, \quad \tau_3 = -1, \quad \tau_5 = \frac{\hbar^2}{16m^2}, \tag{3.9}$$

with all other τ's equal to zero. For the equations studied by Doebner and Goldin, $\tau_1, ..., \tau_5$ are arbitrary, but $\tau_6, ..., \tau_{12}$ are zero.

Some of the equations discussed by Puszkarz,[5] belong to the class (2.15), when $\mu_{12} = 0$. Puszkarz's modification of the Schrödinger equation is the formal extension of the equations of Doebner and Goldin obtained by modifying the current (2.6), adding to it any or all of the following terms with higher derivatives:

$$\rho\triangle(\frac{\mathbf{j}}{\rho}), \quad \rho\nabla(\frac{\mathbf{j}\cdot\nabla\rho}{\rho^2}), \quad \rho\nabla(\frac{\mathbf{j}^2}{\rho^2}), \quad \rho\nabla R_2, \quad \rho\nabla R_5.$$

Since Puszkarz's modification directly affects only the imaginary part of the nonlinear functional for $i\frac{\partial\psi}{\partial t}/\psi$, namely $(-1/2\rho)\nabla\cdot\mathbf{J}$ where $\mathbf{J}$ is the current that appears in the equation of continuity, and does not change the real part, the resulting equation is 4th-order. Our equations are in general 6th-order because of the term with R_{12}, which is needed in order to maintain invariance under the nonlinear gauge group. The equations of Puszkarz with the first three currents do not belong to any family that is closed under a group of weakly local nonlinear gauge transformations, since the transformations giving rise to those currents involve derivatives of the phase S. His equations with the latter two currents belong to the family obtained from (2.15) through gauge generalization.

In short, we have obtained a natural family of 6th-order partial differential equations invariant (as a family) for nonlinear gauge transformations of Bäcklund type, that includes a subclass gauge equivalent to the linear Schrödinger equation, a wider subclass gauge equivalent to the equations that Doebner and Goldin studied, and another subclass that intersects the family of equations proposed by Puszkarz. Given a particular equation in our family, we can calculate the 12 gauge-invariant parameters, and from these immediately determine whether the equation is physically equivalent to the free Schrödinger equation or an equation of Doebner-Goldin type, and whether it is Galilean and/or time-reversal invariant.

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